§23. Study of Quantum Spin Systems by Large-Scale Parallel Calculations

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It is well known that magnetism of insulating materials is described by an assembly of interacting quantum spins. In such a system, strong quantum effect often induces a nontrivial wavefunction. However, a precise analysis of such systems is difficult because they are typical many-body problems. Under circumstances, computational methods are very useful to understand the systems more deeply. Each method has not only merits but also demerits at the same time. Thus, frustrated systems in dimensions that are larger than one are quite difficult cases to study. The quantum Monte Carlo simulations face with a so-called negative sign problem when one uses this method in studies of frustrated systems. On the other hand, the density matrix renormalization group method is powerful for one-dimensional cases although the effective applications to systems in dimensions larger than one are now developing. The numerical diagonalization method based on the Lanczos algorithm is an available and feasible way. Unfortunately, available system sizes are limited to being very small. To overcome this disadvantage in numerical diagonalization studies and to obtain useful information about frustrated systems in two dimensions, we have developed an MPI-parallelized code of Lanczos diagonalization. We use the code to carry out calculations of the Lanczos diagonalization.

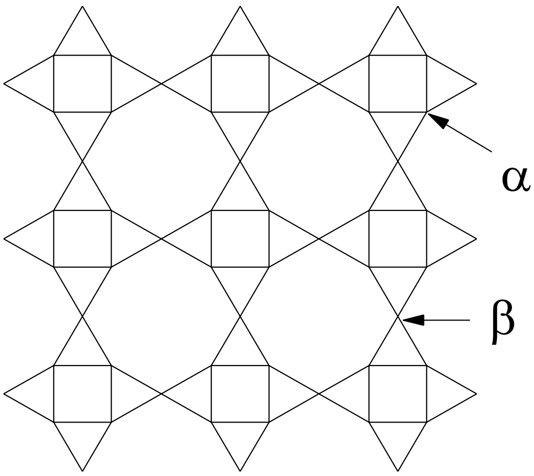

Fig. 1: Square-kagome lattice. There are two types of vertices illustrated by α and β.

In the fiscal year of 2013, we study the magnetization process of the $S = 1/2$ Heisenberg antiferromagnet on the square-kagome lattice[1]. The Hamiltonian of this model is

$$\mathcal{H} = J \sum_{\langle i,j \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j, \quad (1)$$

where $\langle i,j \rangle$ denotes the summation running over all the nearest-neighbor pairs on the square-kagome lattice. This lattice is illustrated in Fig. 1. The square-kagome lattice is similar to the conventional kagome lattice that is composed of small regular triangles connecting each other in a rule of vertex-sharing. The square-kagome lattice is also composed of triangles with the same rule of vertex-sharing, but the network is slightly different from the conventional kagome lattice. Due to this difference, there are two kinds of vertices in the square-kagome lattice while all the vertices are equivalent in the conventional kagome lattice. We examine what happens in the existence of the difference in a lattice of vertex-sharing triangles. We find in the magnetization process that the system shows a magnetization plateau at the one-third height of the saturation in its magnetization process; the plateau is accompanied by a magnetization jump at the higher-field edge. In order to clarify the mechanism of the occurrence of the jump, we observe the local magnetization, capturing the behavior of the spin-flop phenomenon in spite of the fact that the system is isotropic in spin space, where the spin-flop phenomenon is widely known to be a phenomenon that occurs when the system includes some anisotropy. The same behavior is observed in the Heisenberg antiferromagnet on the Cairo-pentagon lattice[2].

We have studied quantum spin systems by MPI-parallelized calculations of Lanczos diagonalization; our results contribute much to our understandings of the frustrated systems.

1) H. Nakano and T. Sakai: J. Phys. Soc. Jpn. **82** (2013) 083709.

2) H. Nakano, M. Isoda, and T. Sakai: J. Phys. Soc. Jpn. **83** (2014) 053702.